

Reconstructing equation of state of dark energy with principal component analysis

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Abstract. We represent a method to reconstruct the equation of state for dark energy directly from observational Hubble parameter data in a nonparametric way. We use principal component analysis (PCA) to extract the signal from data with noise. In addition, we modify Akaike information criteria (AIC) to guarantee the quality of reconstruction and avoid over-fitting simultaneously. The results show that our method is robust in reconstruction of dark energy equation of state. Although current observational Hubble parameter data alone can not give a strong constraint yet, future observations with more accurate data can help to improve the quality of reconstruction significantly, which is consistent with the results of H.-R. Yu et al.

Keywords: dark energy, equation of state, observational Hubble parameter, principal component analysis

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1 Introduction

Distance measurements of the type Ia supernovae (SNe Ia) indicate that the expansion of the universe is accelerating [1–3]. This implies that some mechanism must exist to provide a repulsive effect. Many theories have been proposed to explain this repulsive effect. The most popular one is the dark energy scenario. Dark energy is one kind of special matter which can provide the repulsive force that accelerates the expansion of the universe. However, its nature still remains unclear. To study the property of dark energy, Turner and White [4] suggest to parameterize the dark energy by its equation of state, $w \equiv P/\rho$, where P is pressure and ρ is energy density. For different dark energy models, w takes different values (e.g., -1 for vacuum energy, $-N/3$ for topological defects of dimensionality N), and w also can evolve with time (e.g., models with a rolling scalar field). The analysis from the Planck + WP and BICEP2 data shows that the equation of state $w \neq -1$ and the bounce inflation scenario is better than the standard cold dark matter model with a cosmological constant [5, 6]. Although observation is consistent with $\Omega_M < 1$ and a cosmological constant $\Lambda > 0$ [7], the possibility of a time dependence of w or a coupling with cold dark matter cannot be excluded [8]. Current observational data (SNe + WMAP5 + SDSS) also favor a model predicting $w(z)$ crosses -1 in the range of $z \in [0.25, 0.75]$ [9, 10]. In addition, on the theoretical level a constant Λ runs into serious problems, since the present value of Λ is 10^{123} times smaller than the prediction from most particle physics models. If Λ is not a constant, the dynamic properties of the dark energy may interest us [11, 12]. Since w can well describe the dynamic properties of dark energy, it is vital to determine w in the research of dark energy.

To determine the equation of state for dark energy, there are many different observational data sets can be used. CMB anisotropy, supernovae (SNe) distance measurements and number counts all appear to be promising. One can fit directly to SNe magnitudes or their luminosity distances $d_L(z)$, or to more indirect quantities such as dark energy density, $\rho(z)$, the expansion history, $H(z)$ [13]. But even accurate measurements of d_L cannot constrain the small bumps and wiggles that are crucial to the reconstruction of w . Without some amount of smoothing of the cosmological measurements, reconstruction is impractical [12]. As the combination of number counts and supernova measurements could determine $H(z)$ directly and eliminate the dependence of the second derivative of d_L , using observational Hubble parameter data to constrain w seems to be a good choice.

Recently, there have been many works focus on dark energy equation of state reconstruction. Parametric methods and non-parametric methods are two general methods for this issue. Studying dark energy in a parameterized way, i.e., parameterizing the dark energy equation of state in terms of known observables [8], e.g. Chevallier-Polarski-Linder parametrization [14, 15] and divergency-free parametrizations [16], may induce biased results due to prior assumptions of function forms of the equation of state [17]. It is wiser to reconstruct dark energy equation of state with non-parametric ways, since we do not know the nature of the dark energy so far. Reconstruction methods can also be divided into model dependent methods and model independent methods. Model dependent methods work within a particular model, while model independent methods have no such constraint. In fact, any imposition would cause biased results [18], as a consequence of the strong degeneracy between cosmological models [19]. Therefore, a reconstruction of $w(z)$ should be carried out ideally in a model independent manner [20].

In this paper, we apply principal component analysis (PCA), which is an useful non-parametric model-independent tool, on reconstruction of dark energy equation of state with observational Hubble parameter. However, in order to reconstruct $w(z)$ we need to calculate the derivatives in $H(z)$ which can, in general, increase the errors on the reconstructed equation of state factor [17, 21]. To overcome this defect, we try to fit $w(z)$ directly to observational Hubble parameter data through the integral that relates $w(z)$ to $H(z)$. Another problem is that PCA can pick up the principal components in $w(z)$, but how many components one should keep is still an open question. Too many parameters may cause overfitting and vise versa. So we attempt to modify Akaike information criteria (AIC) in order to guarantee the quality of reconstruction and avoid over-fitting.

This paper is organized as follows. First, we describe the reconstruction process of dark energy equation of state in section 2. Next, we explain the generation of simulated data in section 3. After that, we introduce the information criteria for components selection in section 4. Then we show results in section 5. Finally, we discuss the implications of our results and draw the conclusions in section 6.

2 Reconstructing process

We reconstruct the equation of state for dark energy with the assumption that the universe is homogeneous, isotropic and governed by Einstein's theory of gravitation. It is well known that the metric for a space-time with homogeneous and isotropic spatial sections is the maximally-symmetric Friedmann-Robertson-Walker (FRW) metric. We also treat the whole universe as ideal fluid. Then from Friedmann equation we have

$$\frac{H^2(z)}{H_0^2} = \Omega_m(1+z)^3 + \Omega_r(1+z)^4 + \Omega_x e^{3 \int_0^z \frac{1+w_x(z')}{1+z'} dz'} + \Omega_k(1+z)^2, \quad (2.1)$$

where Ω_x is dark energy density component, Ω_m is matter density component, Ω_k is curvature component, and Ω_r is radiation density component respectively. According to the latest result from Plank, we adopt $H_0 = (67.4 \pm 1.4) \text{ kms}^{-1} \text{ Mpc}^{-1}$, $\Omega_x = 0.6825$, $\Omega_m = 0.3175$, $\Omega_k = 0$, $\Omega_r = 0$ [22]. Then (2.1) can be reduced to

$$\frac{H^2(z)}{H_0^2} = \Omega_m(1+z)^3 + \Omega_x e^{3 \int_0^z 1+w(z') d \ln(1+z')}, \quad (2.2)$$

from which we can calculate the theoretical Hubble parameter $H_{th}(z)$ given an expression for $w(z)$. We can fit observational $H_{ob}(z)$ data to constrain the analytical form of $w(z)$. Through least-square method,

$$\chi^2 = \sum_{i=1}^N \frac{[H_{ob}^i(z) - H_{th}^i(z)]^2}{\sigma_i^2}, \quad (2.3)$$

where N is the number of data points, H_{ob} is observational or simulated Hubble parameter data, H_{th} is theoretical Hubble parameter, and σ is the error of H_{ob} respectively. However, as we have known, simply applying Least-square minimization can not distinguish between noise and signal, as noise is included in the result of optimization. In order to minimize the effect of noise, we use PCA to pick up the principal components of $w(z)$.

The process of applying PCA on reconstruction of equation of state is described as follows: Step 1. We choose a set of basis functions $f_i(z)$, which are orthotropic and complete, and equation of state $w(z)$ can be expressed as

$$w(z) = \sum_{i=1}^N \alpha_i f_i(z), \quad (2.4)$$

where α_i are the coefficients of the corresponding basis functions. Step 2. We use (2.2) and Least-square optimization to derive the coefficients α_i , so we can obtain a distribution of α with enough running of step 2. Step 3. We calculate the covariance matrix of α , denoted by C . Step 4. We calculate the eigenvalues λ_i and eigenvectors by diagonalizing the covariance matrix C ,

$$C = E \Lambda E^T, \quad (2.5)$$

where Λ is the diagonal matrix. The diagonal entries of Λ are eigenvalues, and the columns of matrix E are corresponding eigenvectors. Then we define a new basis $U = FE$, where $F = (f_1, f_2, \dots, f_N)$. This new basis is also orthotropic and complete as a linear combination of the original basis functions f_i , and u_i satisfies

$$Var(u_i) = \lambda_i, i = 1, 2, \dots, N. \quad (2.6)$$

The u_i s with small variance are the relatively stable components, which vary little for different observations. They are hence the components we need.

Step 5. We sort the components by λ_i in ascending order and choose first M components to reconstruct $w(z)$. Besides, a criteria is needed to decide how many components should be used, which will be discussed in section 4.

Step 6. We use new basis functions and Least-square Optimization to fit $H(z)$ data again and obtain the new coefficients. Finally we get equation of state

$$w(z) = \sum_{i=1}^M \beta_i u_i(z), \quad (2.7)$$

where β_i are the new coefficients derived by Least-square Optimization, and M is the number of used components.

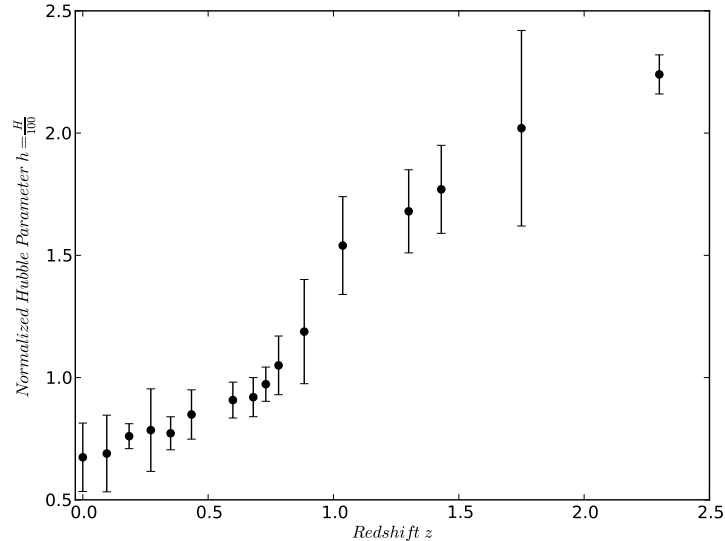


Figure 1. Binned observational Hubble parameter data. Black dots are binned observational Hubble parameter, which extend to $z = 2.3$. The bars show the deviation of Hubble parameter data, which is used to build an error model for the generation of simulated Hubble parameter data.

3 Generation of simulated data

In order to validate the reconstruction process described in section 2, we use the simulated Hubble parameter data set, generated from some toy models (with known $w(z)$), to reconstruct the equation of state. Then we can evaluate the quality of reconstruction through comparing reconstructed equation of state with the known $w(z)$.

We generate simulated Hubble parameter data based on observational hubble parameter data set. Current observational hubble parameter data are obtained primarily from the method of cosmic chronometers [23–26]. Other methods to extract $H(z)$ are by the observations of BAO peaks [27, 28] and Ly- α forest of luminous red galaxies (LRGs) [29], which has extended the current OHD up to $z = 2.3$. Ref.[30] provides the data set we use, which covers several independent measurements of $H(z)$. There are 29 data points in the data set in total (H_0 included). As the redshift distribution of these data points is not (even not close to) an uniform distribution, we split the redshift region ($0 < z < 2.3$) into 15 bins. The binned observational Hubble parameter data set is shown in figure 1.

To generate a simulated Hubble parameter data set, we need a fiducial model which can be characterized by an equation of state $w(z)$, from which we can get the theoretical Hubble parameter H_{th} via (2.2) with a particular $w(z)$. In addition to the underling model, we also need an error model, which estimates the deviations for simulated Hubble parameter data from the theoretical values. There have been some studies on how to obtain an error model from observational Hubble parameter data, for instance, in [17] Yu et al. suggested that the error of observational Hubble parameter data follow Nakagami m distribution; C.M. used the center line of upper heuristic bounds and lower heuristic bounds of the observational Hubble parameter data as the error model for simulated Hubble parameter data in [31]. If the uncertainty of the observational data is strongly dependent on redshift, we can fit the error of

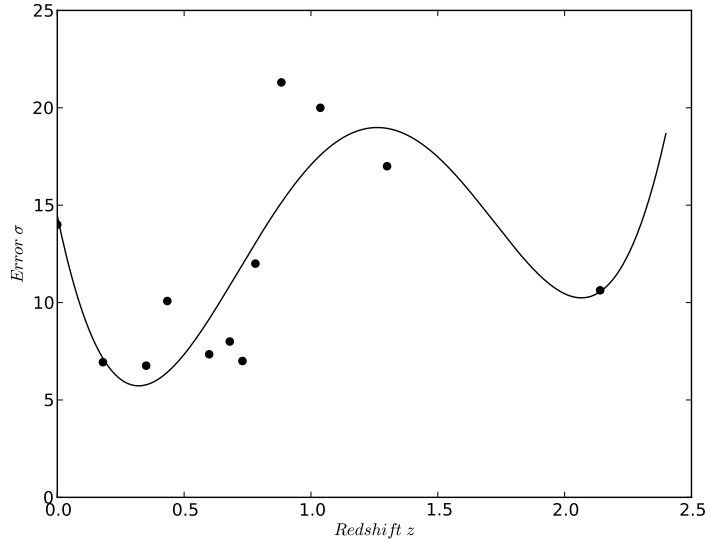


Figure 2. Error model obtained from the observational Hubble parameter data. The curve is obtained through polynomial fitting to the error of binned observational Hubble parameter data. The error of binned observational Hubble parameter data is plotted as the black dots.

the observational Hubble parameter data. The error model for simulated Hubble parameter data we obtained from the observational Hubble parameter data is shown in figure 2.

Finally, with the fiducial model and the error model discussed above, we can generate the simulated Hubble parameter data via

$$H_{sim}(z) = H_{th}(z) + G(0, \sigma(z)), \quad (3.1)$$

where $\sigma(z)$ is the error function, $G(\mu, \sigma)$ is the Gaussian distribution, μ is the mean of the distribution and σ is the standard deviation of the distribution respectively.

4 Criteria for components selection

We have discussed the reconstruction process in section 2. However, the reconstruction is not complete. We need a criteria to determine how many components we should keep in the reconstruction. In this section, we introduce the criteria we used for components selection.

The number of components should be kept is still an open question in principal components analysis. Many criteria have been proposed to solve this problem since PCA was invented in 1901, e.g. Akaike information criteria (AIC), Bayesian information criteria (BIC) [32], and the combinations of them. Yu et al. used a criterion called Goodness of Fit [17]. Although these criteria works well in general, there are defects in these criteria: introducing either additional parameter or additional assumptions, such as s in the combination of AIC and BIC [33]. Furthermore, evaluating these parameters arbitrarily may lead to quite different reconstructing results in some particular problems.

In this paper, we introduce a criteria based on AIC. As there are dozens of data points, we replace AIC with AICc (the small-sample-size corrected version of AIC). The expression of AICc is

$$AICc = \chi_{min}^2 + (\frac{2N}{N - M - 1})M, \quad (4.1)$$

where M is the number of parameters, i.e. the number of components we keep, and N is the size of data set, χ_{min}^2 represents the deviation from observational data or simulated data. It is expected that reducing M will be accompanied by a reduction in the error, but an increased chance of getting $w(z)$ wrong [33], which means $w(z)$ is reconstructed less accurately (so the bias increases), but the error bars are smaller (so the variance decreases)[34]. It turns out that the challenge for this issue is to achieve a balance between the bias and variance. Therefore we add an empirical parameter s into the latter item of AICc to determine the value of s . After that, the modified AICc criteria is

$$AICc = \chi_{min}^2 + s(\frac{2N}{N - M - 1})M, \quad (4.2)$$

where s is the tuning factor we add to AICc to include the penalty for more parameters and to avoid overfitting.

The value of s is determined empirically and consists with the fact that results of best fit have the minimum AICc values. In practice, we use reconstruction results of different models to constrain s . As already known the fiducial model, we can choose proper number of components according to Max Likelihood Estimation. The joint distribution of data points follows chi-square distribution, so the likelihood function can be expressed as

$$\mathcal{L} = \exp(-\chi^2), \quad \chi^2 = \sum_{i=1}^N \frac{(w_i - \mu_i)^2}{\sigma_i^2}, \quad (4.3)$$

where w is the reconstructed equation of state, and μ is the underling equation of state with error σ . When we choose a set of components generated by PCA, we can calculate the associated χ^2 . When χ^2 reaches the minimum, i.e. the likelihood function achieves the maximum, the corresponding set of components are what we need in the final reconstruction. Once the number of components is fixed, we can calculate the AICc to constrain s and further determine the value of s . For a given s , we can apply the AICc criteria on components selection. In other words, we should pick up proper number of components to make the AICc achieve the minimum.

5 Results

Following the reconstruction process described in section 2, in this section we reconstruct the equation of state from simulated Hubble parameter data generated from the fiducial model (with pre-set equation of state $w(z)$). The error of the simulated Hubble parameter data is 20% of that of observational Hubble parameter data. There are three $w(z)$ we reconstruct: a. Λ CDM model, $w(z) = -1$; b. model-1, $w(z) = -\tanh(\frac{1}{z})$; c. model-2, $w(z) = -1 + [1 - \tan(\frac{1}{z})] \sin z^{2.5}$. Their equations of state are shown in figure 3.

The results of reconstructions are shown in figure 4. It is evident that the reconstruction is reliable. Pre-set $w(z)$ s are well in 1σ regions of reconstructed $w(z)$ s. Furthermore, the reconstructed $w(z)$ well shows the variation trends of pre-set $w(z)$ s. In terms of variance, we can see the variances of reconstructed $w(z)$ s are under control at $0 < z < 2.0$. But at $z > 2.0$, the variances dramatically increase. The right panel in figure 4 shows that the Hubble parameter (to be convenient, we draw $H(z)/(1+z)$ instead of $H(z)$) calculated from

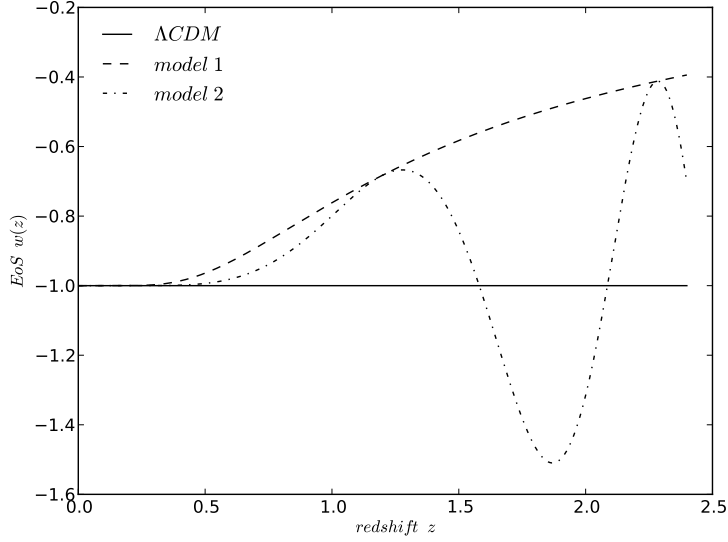


Figure 3. Equation of state for three models. Solid line shows the equation of state of Λ CDM model, dash line shows the equation of state of model-1, and dash-dot line shows the equation of state of model-2. For model-1, $w(z)$ is -1 at present and approaches to 0 as redshift increases. For model-2, $w(z)$ oscillates around -1 with an amplitude increases from 0 to 1.

reconstructed $w(z)$ is consistent with the Hubble parameter obtained from pre-set $w(z)$ s. And the orange region is narrow, which implies that the variance of reconstructed Hubble parameter is very small.

After reconstructing the equation of state for the fiducial models, we obtain the optimum value of s , using the method described in section 4. Then we apply the modified AICc criteria to reconstruct the equation of state from the Hubble parameter data with current error level. We follow the same process to reconstruct $w(z)$ from simulated Hubble parameter data (with underlying model-1). The error level of simulated Hubble parameter data is similar to that of the observational Hubble parameter data. The results are shown in figure 5. We can see that the reconstructed $w(z)$ of simulated Hubble parameter data (with model-1) closely follow the underlying $w(z)$, as shown by $w_{model-1}$, at $0 < z < 1.5$. While the reconstructed $w(z)$ of simulated Hubble parameter (with model-1) deviates from $w_{model-1}$ rapidly at $z > 1.5$. And the variance of the reconstructed $w(z)$ is large. We hence conservatively conclude that the reconstruction is robust at $0 < z < 1.0$. We also show $w(z)$ reconstructed from the observational Hubble parameter data without model, as w_{reco} . Compared to the reconstructed $w(z)$ of the simulated Hubble parameter data (with model-1), w_{reco} oscillates more wildly. The right panel in figure 5 shows the reconstructed Hubble parameter. It is clear that although the Hubble parameter calculated from the reconstructed $w(z)$ of simulated Hubble parameter data (with model-1) is consistent with the theoretical Hubble parameter of model-1, its variance is very large. Figure 5 also shows the Hubble parameter calculated from w_{reco} , which is out of 1σ region of Hubble parameter calculated from reconstructed $w(z)$ of the simulated Hubble parameter data (with model-1) and deviates largely from real observational Hubble parameter data.

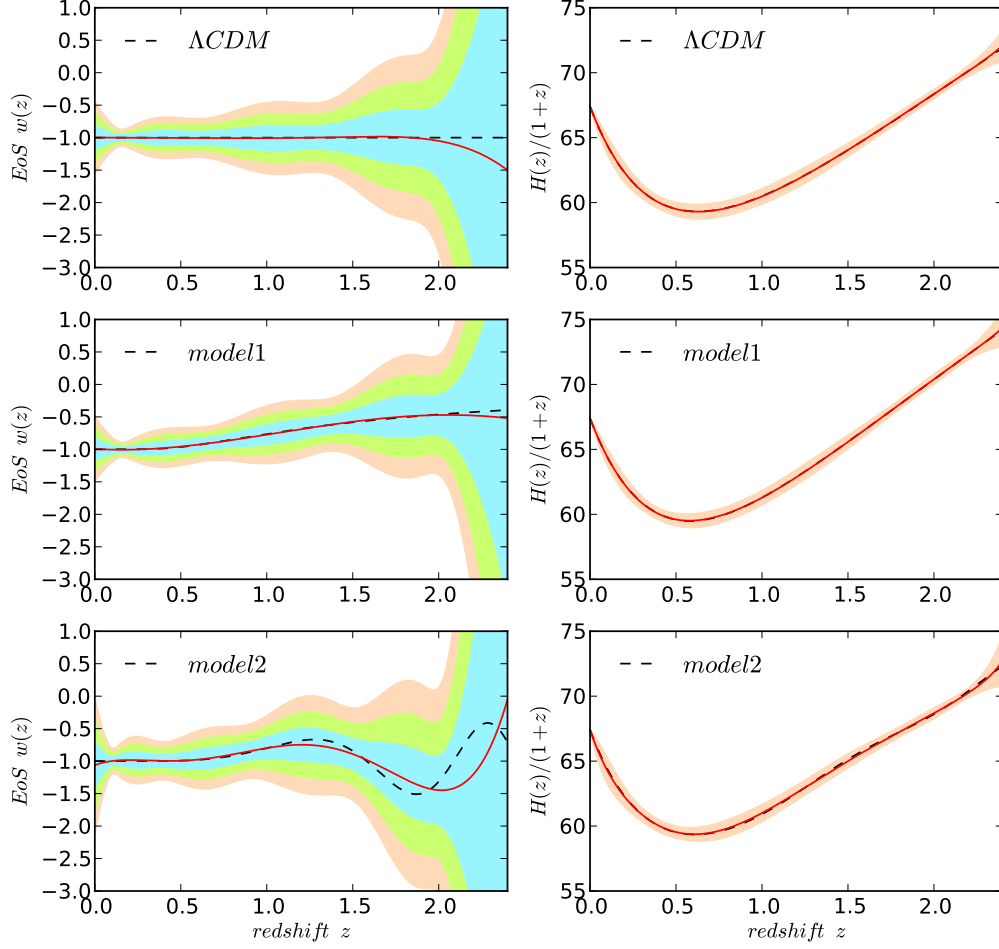


Figure 4. (color online). Left column: Reconstructed $w(z)$ for different models. The light blue shade, green shade and orange shade shows 1σ , 2σ and 3σ error respectively. Black dash line is pre-set $w(z)$, and red solid line shows the reconstructed $w(z)$. Right column: Hubble parameter $H(z)/(1+z)$. Red solid line is the Hubble parameter calculated from the reconstructed $w(z)$. The orange shade shows its 1σ error, and black dashed line shows the Hubble parameter calculated from pre-set $w(z)$.

6 Conclusion and discussion

We apply principal component analysis to reconstruct the dark energy equation of state. We represent $w(z)$ as linear combination of a set of orthogonal basis functions to avoid information loss. In addition, we modify Akaike information criteria (AIC) to balance between bias and deviation in the reconstruction. Then we reconstruct the equation of state for three models from simulated Hubble parameter data (the error is 20% of current observations' error level) to validate our reconstruction process. The results show that we can constrain the equation of state quite well at $0 < z < 2.0$ and the Hubble parameter calculated from reconstructed $w(z)$ is consistent with the Hubble parameter calculated from pre-set $w(z)$ very well as the 1σ

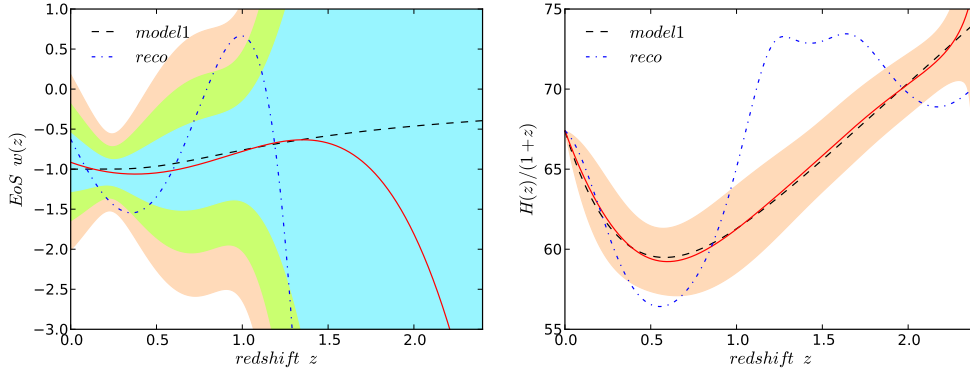


Figure 5. (color online). Left: Red solid line is the reconstructed $w(z)$ of simulated Hubble parameter data (with model-1). The light blue shade, green shade and orange shade shows 1σ , 2σ and 3σ error respectively. Black dashed line is $w(z)$ of underlying model, and blue dash-dot line shows the reconstructed $w(z)$ of the observational Hubble parameter data (with no underlying model). Right: Red solid line is the Hubble parameter calculated from the reconstructed $w(z)$ of simulated Hubble parameter data (with model-1), with orange shade of 1σ error. Black dash line shows the Hubble parameter calculated from $w(z)$ of underlying model, and blue dash-dot line shows the Hubble parameter calculated from the reconstructed $w(z)$ of the observational Hubble parameter data (with no underlying model).

region is very narrow. However, differences of the Hubble parameter derived from different models are very small, although the models are quite different. This is also the reason why reconstructing dark energy equation of state from Hubble parameter data is difficult. Nevertheless, from this study we show that future observations with 20% error of current observational data will help to constrain dark energy equation of state to redshift $z \simeq 2.0$. We confirm that future observations with larger quantity and better quality will greatly improve the reconstruction of dark energy [17] and a small sample collected at much higher redshift will reduce the errors more efficiently than collecting more events in the original redshift interval [35].

In the case of reconstructing dark energy equation of state from real observational Hubble parameter data, we can constrain $w(z)$ at $0 < z < 1.0$ with an underlying model. But the reconstructed $w(z)$ deviates largely from $w(z)$ of underlying model at $z > 1.0$, as the quality of data is very poor. If there is no underlying model, the reconstructed $w(z)$ oscillates even more wildly, and we can not know whether it is close to the true $w(z)$.

Since we do not understand the nature of dark energy, it is possible that dark energy can lead to other observable effects such as a new long range force [36]. More accurate observations are needed to reveal the secrets of dark energy.

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